

Molecular dynamics simulation on notch sensitivity of nanocrystalline Cu

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A molecular dynamics (MD) simulation was performed on the nanocrystalline (NC) Cu with an edge notch under tensile loadings, with focus on the notch sensitivity. With the increase of notch size, the dominant deformation of material changes from the shear strain, which spreads throughout the entire sample, to a single shear band, which is induced by the stress concentration at the notch root. At the same time, the samples move from notch-insensitivity to notch-sensitivity. These findings offer significant guidelines for the application of NC Cu in engineering.

1. Introduction: Nanomaterials have attracted considerable interest due to their extraordinary physical properties since the discovery in the 1980s [1–3]. For an engineering material, understanding its failure mechanism is very necessary as it plays a significant role in engineering structure and the reliability of the equipment. The various inevitable defects shall nucleate and transmit in materials, and finally cause the failure. If the defect sensitive of a material is relatively low, it can contain more defects and hold the edge in engineering application. The notch is the most common defect form of the materials. Due to this, studying the failure mode of nanometre materials, especially the notch sensitivity, has become a hot topic [4–7].

Tensile testing is one of the most common methods to detect the material notch sensitivity. According to previous studies, different materials have different degrees of sensitivity to the notch, such as metallic glass [5], nanoglass [4], nanocrystalline (NC) graphene [6] and other materials [7]. However, the problem of NC material's notch sensitivity has not been studied. We do not know whether the presence of the notch affects the failure mode of the NC metals. Also, what is the impact of the notch on the failure of the NC metal? Also, how does the notch affect the failure mechanism? So it is very important and necessary to understand the effect of the notch on the failure behaviours of NC materials. Nano-Cu is a new hot metal, it can be widely applied in microelectronic components and coating. To make a deep understanding of the nanometal, in this Letter, molecular dynamics (MD) simulations (MD) [8] will be used to study the notch sensitivity in NC Cu with grain size $d = 5$ nm.

2. Simulation: All MD simulations which adopt the software Large-scale Atomic/Molecular Massively Parallel Simulator [9, 10] with an integration time step of 5 fs were performed on the NC Cu. The dimensions of the Cu sample are $50 \times 25 \times 4$ nm³, containing $\sim 420,000$ atoms in a section of Cu film. An embedded atom method inter-atomic potential [11] for NC Cu was adopted. Periodic boundary conditions were applied in the X -axis. To relax the atomic structure of the interfaces and eliminate voids, each sample was equilibrated at 300 K under isothermal-isobaric ensemble (NPT, normal pressure and temperature) for 100 ps before the deformation. After reaching a stable system, in the x -direction, a constant strain rate of 109 s^{-1} was applied to simulate the tensile tests at 300 K. To study the impact

of notch size on the failure mode of the NC Cu, four different simulation samples were constructed with the diameter (D) of notch ranging from 2 to 15 nm and facing the positive direction of the Y -axis. Also, a three-dimensional (3D) model of samples is shown in Fig. 1.

A visualisation tool OVITO [12] was used to visualise the data of simulation and analyse it. With the technique of common neighbour analysis (CNA), notch defects were visualised.

3. Results and discussion: Stress–strain curves for NC Cu with different sizes of notches in samples are shown in Fig. 2. To show the influence of notch size on the samples clearly, the stress–strain curves for NC Cu without a notch and NC Cu with notches of $D = 2$ and 5 nm are displayed in Fig. 2a. Fig. 2b shows the stress–strain curves for notch-free NC Cu and notched NC Cu with $D = 10$ and 15 nm under tension loading. For Fig. 2a, the notch diameter (D) of the samples is less than or equal to the average diameter (d) of Cu grains. In contrast, Fig. 2b depicts the D is greater than d in diameter. By comparing Fig. 2a with Fig. 2b, it is evident that the three curves have extremely strong similarity in movement when $D \leq d$. When the stress reaches the maximum value, which is about 2.5 GPa at a strain of 6%, the stress fluctuates up and down with the increase of the strain without obvious decrease. However, when $D > d$, the maximum value of the stress is < 2.5 GPa, and the stress drops rapidly after reaching the maximum value until it drops to zero.

Fig. 1 shows a sequence of images of the atomic deformation processes at a strain of 2%, 7%, and 15%, respectively, for NC Cu with notch-free, notch sizes $D = 2$ and 5 nm. It is obvious that the deformation of the specimens is similar. It is noted that the atomic local shear strain [13, 14] begins to appear locally in the samples at a strain of 7%, and the shear strain increases and gradually spreads throughout the samples when the strain reaches 15%. However, these shear strains are randomly dispersed throughout the sample instead of focusing on a fixed area, and the size of the strain localisation is relatively similar, without significant difference. Therefore, the deformation of the material is similar under tensile and is irrelevant to the notch. Fig. 1 indicates that when $D \leq d$, the failure of NC Cu is insensitive to the notch.

It should be emphasised that when the notch size D is smaller than or equal to the grain size d , the insensitivity of the Cu to the notch has nothing to do with the location and shape of the

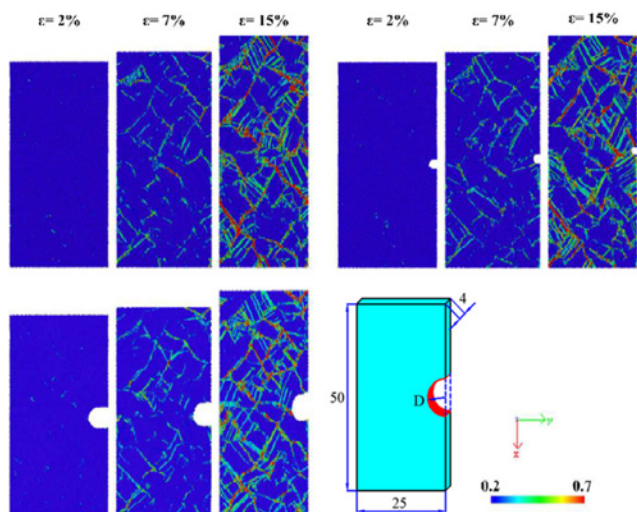


Fig. 1 Sequence of images which describe the atomic deformation processes for NC Cu with notch-free, notch size $D = 2$ nm and 5 nm

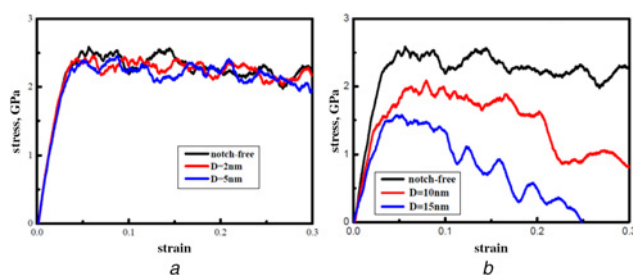


Fig. 2 Stress-strain curves of different samples
a Stress-strain curves that indicate samples of NC Cu without a notch and with notch sizes $D = 2$ and 5 nm ($D \leq d$)
b Stress-strain curves for samples without a notch and with notch sizes $D = 10$ and 15 nm ($D > d$)

notches. As shown in Figs. 3*a* and *b*, the stress-strain curves and atomistic configurations do not change significantly when the shape and position of the notch are changed.

Fig. 4 shows a sequence of snapshots that describe the deformation process for NC Cu samples with $D = 10$ and 15 nm. In Fig. 4, it can be seen that the plastic zone appears at the root of the notch in the early stage of plastic deformation ($\epsilon = 3.8\%$), and the shear strain mainly appears at the grain boundaries. Nevertheless, the macroscopic deformation of the sample is still similar. As soon as the strain reaches 8.2%, corresponding to the position of the first major stress that drops in Fig. 2, a single dominant shear band, i.e. 45° to the tensile direction, is formed when the plastic zone propagates across the sample. By comparing these frames, it is found that the shear band becomes more and more obvious as the strain increases until the sample breaks at a strain of 24.8%. Meanwhile, the stress-strain curve is also reduced to zero. The overall trend of the stress-strain curve is declined during the tension process, which indicates that the failure mode of the sample is dominated by the slip of the shear band. At the same time, the initial plastic zone occurs at the notch root and spreads to the sample subsequently. That is the reason for the form of the single dominant shear band, which leads to the failure of the sample. Therefore, the failure behaviours of the sample have some connection with the notch and the location of the notch. Fig. 4 shows that when $D > d$, the failure of NC Cu is sensitive to the notch.

In conclusion, the simulation results show that the sensitivity of the NC Cu with the grain diameter of 5 nm is related to the size of

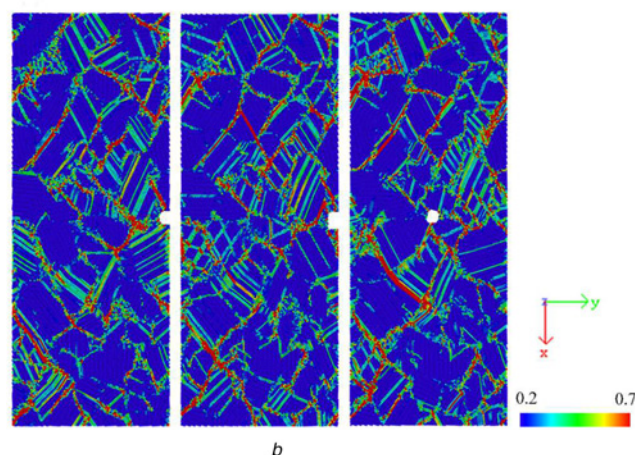
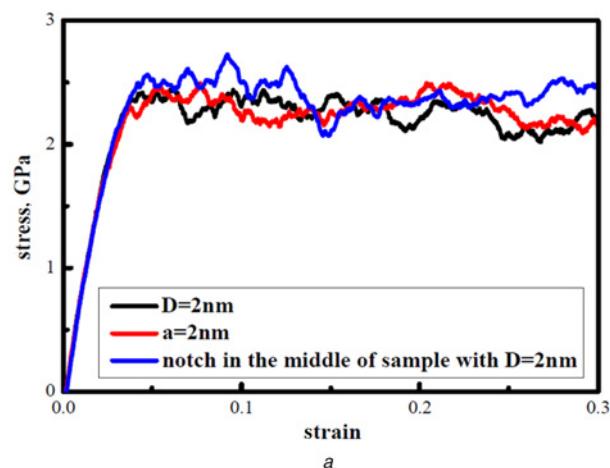


Fig. 3 Samples with a notch in different positions or notch of different shapes

a Stress-strain curves for samples of NC Cu with notch sizes D or $a = 2$ nm
b Sequence of snapshots capturing the atomic deformation processes at a strain of 15% for NC Cu

the notch. When the notch size D is smaller than or equal to d , the macroscopic deformation of the sample is homogeneous, similar to the deformation of the sample with notch-free, and the Cu shows notch insensitivity. This result illustrates that the deformation of samples has nothing to do with the stress concentration at the notch root. On the contrary, when $D > d$, the initial strain concentration appears at the notch root and subsequently propagates across the sample during the tension, which leads to the formation of a dominant shear band that penetrates the sample and causes the sample failure. The Cu shows notch sensitivity. The results indicate that the formation of shear bands is caused by the stress concentrated at the notch root [15]. Therefore, there is no denying that stress concentration is an important factor affecting the notch sensitivity of NC Cu.

It is well known that stress concentration occurs at the notch root during the tension process, and the stress at the root is greater than the average stress of the sample. As shown in Fig. 2, when the notch size $D \leq 5$ nm, the maximum stress of the sample is about 2.5 GPa, close to the stress of sample without a notch, which is the yield stress of the material. At this time, the stress concentration at the notch root, and the maximum stress is greater than the yield stress. Therefore, the shear strain, which spreads throughout the samples by distributing in the atomic interfaces, causes the homogeneous deformation. When the notch size is 15 nm, the maximum stress of the specimen is about 1.5 GPa, which is lower than the yield stress of the material. As a result, shear strain

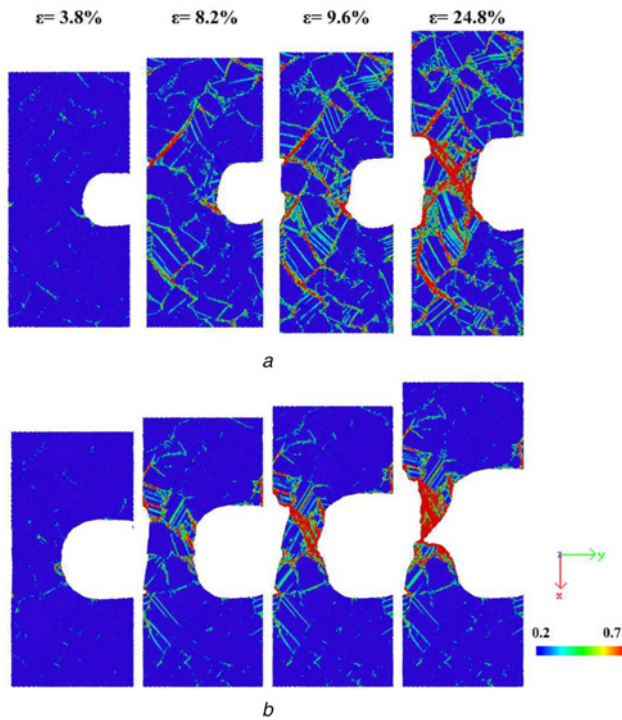


Fig. 4 Sequence of images describing the atomic deformation processes for NC Cu with notch size $D = 15$ nm

accumulates in the notch root, instead of spreading throughout the sample. When the plastic strain region size reaches a critical value, a dominant shear band is initiated from the notch root [5] and then passes through the entire sample, resulting in material failure [16].

For a deeper understanding, the deformations of grains were discussed. During the deformation, the relative displacement between atoms is shown in Fig. 4b. Different colours are shown in the picture because of the different relative displacement of atoms, which causes the change of local von Mises shear strain.

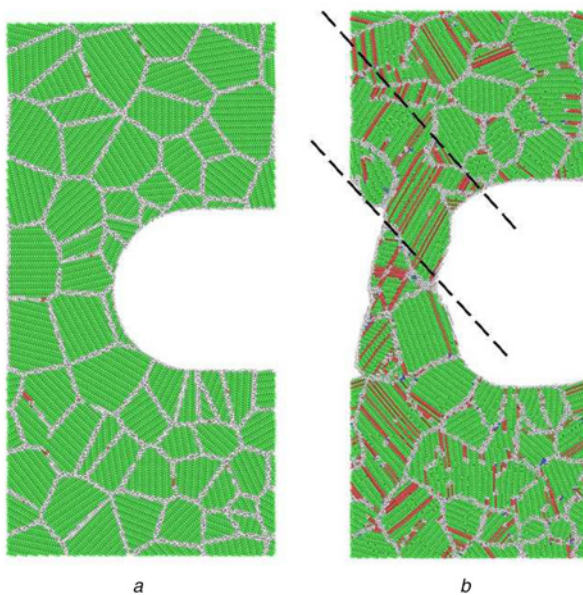


Fig. 5 Grain structure of the NC Cu sample with $D = 15$ nm, coloured according to CNA

a Initial structure before straining
b In the strain localisation region, grains merge into one, which is marked with dashed black lines

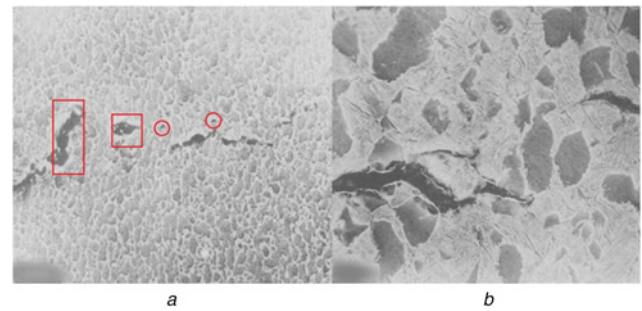


Fig. 6 SEM pictures [24]

a Nano-voids and micro-cracks
b Process of the main crack link up voids

Therefore, the function of these figures is to record the local material deformation process and the dislocation movement trajectory. From Fig. 4b, we can see that in the process of the strain increase, the bright blue in the figure gradually becomes dark red, which shows that the relative displacement of the atoms during the stretching process has changed. The deepening of the colour indicates that there are a new dislocation emission and expansion at the position, which is nucleation and emission of partial dislocations [17–19].

By comparing Fig. 5a with Fig. 5b, we can find that the grains are much easier to grow and merge during the tension progress. It agrees with the previous experiment results [20–22]. The grain growth, which is the result of a series of grain boundary migration and coarsening phenomenon caused by grain rotation, is closely related to high-shear stress that the materials receive during deformation [23]. However, the need to pay attention to is that grain deformation is not obvious in the region far away from the strain localisation, i.e. to say, the plastic deformation of NC Cu occurs mostly in the grain boundary and inter grain that is close to the strain localisation region. These phenomena explain the reason for the shear band to appear at the notch root from the angle of grain deformation.

Figs. 6a and b [24] show the scanning electron microscopy (SEM) picture of nanovoids nucleate in front of micro cracks. With the increase of strain, nanovoids will expand into micro cracks and be linked up by main cracks. If treating $D \leq d$ notch as nanovoid and $D > d$ notch as micro crack, then our result can be explained in another way. Notches will absorb stress concentration and expand. When $D \leq d$, notch mainly absorb stress concentration to transform into micro cracks. Else, the notch is most likely to expand, so the stress concentration will finally form the slip bands.

4. Summary: To study the notch sensitivity of NC Cu with an average grain size of $d = 5$ nm, the deformation mechanism of NC Cu samples during the tension process is investigated by MD simulations. The simulation results show that the sensitivity of the NC Cu is related to the size of the notch. When $D \leq d$, with shear strain spreading throughout the samples similarly, the deformation of the sample is homogeneous. So, the failure behaviour of NC Cu is irrelevant to the location and shape of the notches. At the same time, the notched Cu shows notch insensitivity. On the other hand, when $D > d$, the deformation of the samples is dominated by the shear band, which is caused by the stress concentration at the notch root. Therefore, the failure of NC Cu becomes notch-sensitive and the failure mode switches to shear banding. These findings contribute to the guideline for the scientists to research the application of NC Cu in engineering.

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6 References

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